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Abstract

In this paper, we study the set of the invariant probabilities of the Vlasov-Fokker-Planck equation. This is a nonlinear diffusion, since the own law of the process intervenes in the drift. In order to make our study, we are lying on the recent results by Tugaut and coauthors about the McKean-Vlasov diffusion. Indeed, we show here that the set of invariant probabilities of the Vlasov-Fokker-Planck equation is related to that of the McKean-Vlasov diffusion.

Keywords:
Invariant measure, Vlasov-Fokker-Planck equation, McKean-Vlasov equation, stochastic processes.
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1. Introduction

1.1. The Vlasov-Fokker-Planck equation

We consider the following *Vlasov-Fokker-Planck (VFP)* equation,

$$\partial_t \rho = -\operatorname{div}_q \left(\rho \frac{p}{m}\right) + \operatorname{div}_p \left(\rho(\nabla_q V + \nabla_q \psi * \rho + \gamma \frac{p}{m})\right) + \gamma k T \Delta_p \rho. \qquad (1)$$

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In this equation, the spatial domain is $\mathbb{R}^{2d}$ with coordinates $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$. The unknown is a time-dependent probability measure $\rho\colon [0,T] \to \mathcal{P}(\mathbb{R}^{2d})$. Subscripts as in div_q and Δ_p indicate that the differential operators act only on those variables. The functions $V = V(q)$ and $\psi = \psi(q)$ are given. The convolution $\psi * \rho$ is defined by $(\psi*\rho)(q) = \int_{\mathbb{R}^{2d}} \psi(q-q')\rho(q',p')\, dq'dp'$. Finally γ, k and T are positive constants.

Equation (1) is the forward Kolmogorov equation of the following stochastic differential equation (SDE),

$$\begin{aligned} dQ(t) &= P(t)\, dt, \\ dP(t) &= -\nabla V(Q(t))\, dt - \nabla\psi * \rho_t(Q(t))\, dt - \gamma\, \frac{P}{m}\, dt + \sqrt{2\gamma k T}\, dW(t). \end{aligned} \tag{2}$$

This SDE models the movement of a particle with mass m under a fixed potential V, an interaction potential ψ, a friction force (the drift term $-\gamma \frac{P}{m}\, dt$) and a stochastic forcing described by the d-dimensional Wiener measures W. In this model, γ is the friction coefficient, k is the Boltzmann constant and T is the absolute temperature.

Eq. (1) and system (2) play an important role in applied sciences in particular in statistical mechanics. For instance, it is used as a simplified model for chemical reactions, or as a model for particles interacting through Coulomb, gravitational, or volume exclusion forces, see e.g., [Kra40, NPT84, BD95]. Eq. (1) (and related models) has been studied intensively in the literature by many authors from various points of view, see e.g. [Deg86, BD95, BGM10, DPZ13, DPZ14, Duo15] and references therein. In particular, invariant probabilities of Eq. (1) has been investigated in [Dre87, BGM10] (see also [Duo15]). However, in these papers, the potential V is assumed to be either bounded or globally Lipschitz or convex. As a result, there is a unique invariant probability. In this paper, we show that when the potential V is unbounded, non-convex and non-Lipschitz, of which a double-well potential is a typical example, non-uniqueness and other interesting phenomena such as phase transition can occur. Herein, we characterise the set of invariant probabilities in such a case. Our study is lying on the recent results by Tugaut and co-authors about the McKean-Vlasov diffusion by showing that the set of invariant probabilities of the Vlasov-Fokker-Planck equation is related to that of the McKean-Vlasov diffusion.

1.2. Normalization

We first write (1) in dimensionless form. By setting

$$q =: L\widetilde{q}, \quad p =: \frac{mL}{\tau}\widetilde{p}, \quad t =: \tau\widetilde{t}$$

and

$$V(q) =: \frac{mL^2}{\tau^2}\widetilde{V}(\widetilde{q}), \quad \psi(q) =: \frac{mL^2}{\tau^2}\widetilde{\psi}(\widetilde{q}), \quad \rho(p,q,t) =: \frac{\tau^d}{m^d L^{2d}}\widetilde{\rho}(\widetilde{p},\widetilde{q},\widetilde{t}),$$

where L is the characteristic length scale, and $\tau := \frac{m}{\gamma}$ is the relaxation time of the particle dynamics. Then the dimensionless form of the Vlasov-Fokker-Planck equation is (after leaving out all the tilde)

$$\partial_t\rho = -\operatorname{div}_q\Big(\rho p\Big) + \operatorname{div}_p\Big(\rho(\nabla_q V + \nabla_q\psi * \rho + p)\Big) + \varepsilon\Delta_p\rho. \tag{3}$$

where $\varepsilon := kT\tau^2 m^{-1}L^{-2}$ is the dimensionless diffusion coefficient.

In this paper, we are interested in stationary solutions of Eq. (3), i.e., solutions of the following equation

$$\mathsf{K}[\rho](\rho) = 0, \tag{4}$$

where

$$\mathsf{K}[\mu](\rho) := -\operatorname{div}_q\Big(\rho p\Big) + \operatorname{div}_p\Big(\rho(\nabla_q V + \nabla_q\psi * \mu + p)\Big) + \varepsilon\Delta_p\rho \tag{5}$$

for given $\mu \in L^1(\mathbb{R}^{2d})$. Note that for a given μ, the operator $\mathsf{K}[\mu](\rho)$ is linear in ρ. This can be seen as a linearised operator of $\mathsf{K}[\rho](\rho)$. Under the assumption that V and ψ are smooths, the linearised operator is hypo-elliptic.

1.3. Organisation of the paper

The rest of the paper is organised as follows. In Section 2, we state our assumptions and provide a characterization via an implicit equation for a stationary probability measure of Eq. (4). In Section 3 we present main results of the paper which prove the existence, (non-) uniqueness and phase transition properties of such invariant probabilities.

2. Characterization of invariant probabilities

We now characterize solutions of Eq. (4).

First of all, we consider the following assumption:

Assumption 1. Assumption (V-1): *V is a smooth function and there exists $m \in \mathbb{N}^*$ and $C_{2m} > 0$ such that* $\lim_{||x|| \to +\infty} \frac{V(x)}{||x||^{2m}} = C_{2m}$.

Assumption (V-2): *The equation $\nabla V(x) = 0$ admits a finite number of solution. We do not specify anything about the nature of these critical points. However, the wells will be denoted by a_0.*

Assumption (V-3): *$V(x) \geq C_4||x||^4 - C_2||x||^2$ for all $x \in \mathbb{R}^d$ with $C_2, C_4 > 0$. $||\,.\,||$ denotes the euclidian norm.*

Assumption (V-4): $\lim\limits_{||x|| \to \pm\infty} \mathrm{Hess}\, V(x) = +\infty$ *and* $\mathrm{Hess}\, V(x) > 0$ *for all $x \notin K$ where K is a compact of $\mathbb{R}^d$ which contains all the critical points of V.*

Assumption (ψ-1): *There exists an even polynomial function G on $\mathbb{R}$ such that $\psi(x) = G(||x||)$. And,* $\deg(G) =: 2n \geq 2$.

Assumption (ψ-2): *G and G'' are convex.*

Assumption (ψ-3): $G(0) = 0$.

The simplest example (most famous in the literature) is that $V(x) = \frac{x^4}{4} - \frac{x^2}{2}$ (i.e., V is a double-well potential) and $\psi = \frac{\alpha}{2}x^2$ for some α (i.e., ψ is a quadratic interaction).

Proposition 1. Suppose that Assumption 1 holds. If there exists a solution $\rho_\infty \in L^1 \cap L^\infty$ of Eq. (4) then

$$\rho_\infty(q,p) = Z_\varepsilon^{-1} \exp\left[-\frac{1}{\varepsilon}\Big(\frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\Big)\right], \quad (6)$$

where Z_ε is the normalizing constant

$$Z_\varepsilon = \int_{\mathbb{R}^{2d}} \exp\left[-\frac{1}{\varepsilon}\Big(\frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\Big)\right] dq\, dp. \quad (7)$$

Conversely any measure whose density satisfies (6) is invariant for (3).

Proof. The idea of the proof has appeared in [Dre87], where the authors study the Vlasov-Fokker-Planck equation but with different scaling and assumptions. The proof is divided into two steps.

Step 1. We first consider the linearised equation

$$\mathsf{K}(\rho) := \mathsf{K}[\mu](\rho) = 0, \tag{8}$$

where $\mu \in L^1(\mathbb{R}^{2d})$ is a given. We prove the following assertion: Define

$$A := \Big\{ v : \mathbb{R}^{2d} \to \mathbb{R} \Big| v(\cdot, p) \in C^1(\mathbb{R}^d)\, \forall p \in \mathbb{R}^d; v(q, \cdot) \in C^2(\mathbb{R}^d)\, \forall q \in \mathbb{R}^d; \text{ and } f := v \cdot u^{-1/2} \text{ satisfies } f \in H^1((1+|q|+|p|)\, dqdp), \Delta_p f \in L^2 \Big\}.$$

Then the linearised equation (8) has a unique solution in A given by

$$u(q,p) := C_\varepsilon^{-1} \exp\left(-\frac{1}{\varepsilon}\Big(\frac{1}{2}p^2 + V(q) + \psi * \mu(q)\Big)\right), \tag{9}$$

where C_ε is the normalisation constant so that $\|u\|_1 = 1$.

Indeed, since $-\operatorname{div}_q(up) + \operatorname{div}_p(u(\nabla_q V + \nabla_q \psi * \mu)) = \operatorname{div}_p(up) + \varepsilon \Delta_p u = 0$, it follows that $\mathsf{K}[\mu](u) = 0$. Now assume that Eq. (8) has another solution $v \in A$ and $\|v\|_1 = 1$. Let $f := v \cdot u^{-1/2}$. Since $v \in A$, f satisfies $f \in H^1((1+|q|+|p|)\, dqdp)$ and $\Delta_p f \in L^2$. Moreover, we have

$$\begin{aligned} &-\operatorname{div}_q(vp) + \operatorname{div}_p(v(\nabla_q V + \nabla_q \psi * \mu)) \\ &= u^{1/2}[-\operatorname{div}_q(fp) + \operatorname{div}_p(f(\nabla_q V + \nabla_p \psi * \mu))], \end{aligned}$$

and

$$\begin{aligned} \operatorname{div}_p \Big(vp + \varepsilon \nabla_p v \Big) &= \operatorname{div}_p \Big(vp + \varepsilon \nabla_p (u\, u^{-1/2}\, f) \Big) \\ &= \operatorname{div}_p \Big(vp + \varepsilon (u \nabla_p (u^{-1/2} f) + \nabla_p u \cdot u^{-1/2} f) \Big) \\ &= \varepsilon \operatorname{div}_p \Big(u \nabla_p (u^{-1/2} f) \Big). \end{aligned}$$

Define $\mathsf{Q}f := -u^{-1/2}\mathsf{K}(\mathsf{u}^{1/2}\mathsf{f}) = -u^{-1/2}\mathsf{K}(v)$. Then from the above calculation, we get

$$\mathsf{Q}f = -[-\operatorname{div}_q(fp) + \operatorname{div}_p(f(\nabla_q V + \nabla_p \psi * \mu))] - \varepsilon u^{-1/2} \operatorname{div}_p \Big(u \nabla_p (u^{-1/2} f) \Big).$$

Therefore, by multiplying by f and integrating over $\mathbb{R}^{2d}$, we obtain

$$\begin{aligned}
\langle \mathsf{Q}f, f\rangle_{L^2} &= \frac{1}{2}\int_{\mathbb{R}^{2d}} [\mathrm{div}_p(pf^2) - \mathrm{div}_p(f^2(\nabla_q V + \nabla_p \psi * \mu))]\, dqdp \\
&\quad - \varepsilon \int_{\mathbb{R}^{2d}} u^{-1/2}\, \mathrm{div}_p \left(u \nabla_p (u^{-1/2} f)\right) f\, dqdp \\
&= \frac{1}{2}\int_{\mathbb{R}^{2d}} [\mathrm{div}_p(pf^2) - \mathrm{div}_p(f^2(\nabla_q V + \nabla_p \psi * \mu))]\, dqdp \\
&- \varepsilon \int_{\mathbb{R}^{2d}} \mathrm{div}_p \left(u^{-1/2}[u \nabla_p (u^{-1/2} f)]\right) + \varepsilon \int_{\mathbb{R}^{2d}} u \Big(\nabla_p (u^{-1/2} f)\Big)^2\, dqdp \\
&= \varepsilon \int_{\mathbb{R}^{2d}} u \Big(\nabla_p (u^{-1/2} f)\Big)^2\, dqdp.
\end{aligned}$$

Since $\mathsf{Q}f = 0$, it follows that $\nabla_p(u^{-1/2} f) = 0$, i.e., $u^{-1/2} f = g(q)$ for some function g. Hence $v = u^{1/2} f = u \cdot g(q)$, and $0 = \mathsf{K}(v) = -up \cdot \nabla_q g(q)$. It implies that $\nabla_q g(q) = 0$, i.e., g is a constant. Since $\|v\|_1 = 1$, we obtain that $g = 1$, i.e. $v = u$. In other words, Eq. (8) has u as a unique solution in A and $\|u\|_1 = 1$.

Step 2. Suppose that $\rho_\infty \in L^1 \cap L^\infty$ is a solution of Eq. (4). Therefore, ρ_∞ solves the equation $\mathsf{L}[\rho_\infty](\nu) = 0$. According to **Step 1**, this equation has a unique solution given by

$$\tilde{\nu} = Z_\varepsilon^{-1} \exp\left[-\frac{1}{\varepsilon}\Big(\frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\Big)\right].$$

Hence $\tilde{\nu} = \rho_\infty$, i.e., ρ_∞ satisfies (6). The reverse assertion is obvious. $\square$

3. Main results

In this section, we assume that Assumption 1 is fulfilled.

Theorem 1. *We consider a measure ρ_∞ on $\mathbb{R}^d \times \mathbb{R}^d$. It is an invariant probability for* (3) *if and only if $q \mapsto \int_{\mathbb{R}^d} \rho_\infty(q,p)dp$ is an invariant probability of*

$$dX(t) = -\nabla V(Q(t))\, dt - \nabla \psi * \mu_t(X(t))\, dt + \sqrt{2\varepsilon} dW(t), \tag{10}$$

Proof. Denote by $\hat{\rho}_\infty$ the first marginal of ρ_∞, i.e., $\hat{\rho}_\infty(q) = \int_{\mathbb{R}^d} \rho_\infty(q,p)dp$.

Then (6) becomes

$$\rho_\infty(q,p) = \frac{\exp\left[-\frac{1}{\varepsilon}\left(\frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right]}{\int_{\mathbb{R}^{2d}} \exp\left[-\frac{1}{\varepsilon}\left(\frac{p^2}{2} + V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right] dqdp}$$
$$= \frac{e^{-\frac{1}{\varepsilon}\frac{p^2}{2}}}{\int_{\mathbb{R}^d} e^{-\frac{1}{\varepsilon}\frac{p^2}{2}}\, dp} \times \frac{\exp\left[-\frac{1}{\varepsilon}\left(V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right]}{\int_{\mathbb{R}^d} \exp\left[-\frac{1}{\varepsilon}\left(V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right] dq} \tag{11}$$

It follows that

$$\hat{\rho}_\infty(q) = \int_{\mathbb{R}^d} \rho_\infty(q,p)\, dp = \frac{\exp\left[-\frac{1}{\varepsilon}\left(V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right]}{\int_{\mathbb{R}^d} \exp\left[-\frac{1}{\varepsilon}\left(V(q) + \psi * \rho_\infty(q) - \psi * \rho_\infty(0)\right)\right] dq}.$$

Note that $\hat{\rho}_\infty$ is the stationary measure of the McKean-Vlasov SDE

$$dX(t) = -\nabla V(Q(t))\, dt - \nabla\psi * \mu_t(X(t))\, dt + \sqrt{2\varepsilon} dW(t), \tag{12}$$

where μ_t is the law of $X(t)$. The forward Kolmogorov equation associated to the McKean-Vlasov SDE is given by

$$\partial_t \mu_t = \operatorname{div}[\mu_t(\nabla V + \nabla\psi * \mu_t)] + \varepsilon\Delta\mu_t. \tag{13}$$

□

Thus, the following statements hold true:

Proposition 2. For any $\varepsilon > 0$, there exists an invariant probability.

This is a consequence of Proposition 3.1 in [Tug14b].

Theorem 2. *If both V and ψ are symmetric, there exists a symmetric invariant probability.*

This is a consequence of Theorem 4.5 in [HT10a].

Proposition 3. Here, $d = 1$. We assume that the interacting potential ψ is quadratic: $\psi(x) := \frac{\alpha}{2}x^2$. Let a_0 be a critical point of V such that $\alpha + V''(a_0) > 0$ and

$$\alpha > 2 \sup_{x \neq a_0} \frac{V(a_0) - V(x)}{(a_0 - x)^2} \,. \tag{14}$$

Thus, for all $\delta \in]0\,;1[$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \leq \varepsilon_0$, Diffusion (3) admits an invariant probability ρ_∞ satisfying

$$\left| \int_{\mathbb{R}} \int_{\mathbb{R}} q\rho_\infty(q,p)dqdp - a_0 + \frac{V^{(3)}(a_0)}{4V''(a_0)\left(\alpha + V''(a_0)\right)} \varepsilon \right| \leq \delta\, \varepsilon \,.$$

This is a consequence of Proposition 1.2 in [Tug14a].

Theorem 3. *Here, $d = 1$. We assume that*

$$V(x) = -\frac{|V''(0)|}{2}x^2 + \sum_{p=2}^{q} \frac{\left|V^{(2p)}(0)\right|}{(2p)!} x^{2p} \quad \textit{with} \ \deg(V) =: 2q \,. \tag{15}$$

And, $\psi(x) := \frac{\alpha}{2}x^2$.
Thus, there exists a $\varepsilon_c > 0$ such that:

- *For all $\varepsilon \geq \varepsilon_c$, Diffusion (3) admits a unique invariant probability, which is symmetric.*
- *For all $\varepsilon < \varepsilon_c$, Diffusion (3) admits exactly three invariant probabilities.*

Moreover, ε_c is the unique solution of the equation

$$\int_{\mathbb{R}_+} \left(4y^2 - \frac{1}{2\alpha}\right) e^{(|V''(0)|-\alpha)4y^2 - \sum_{p=2}^{q} \frac{2x^{p-1}\left|V^{(2p)}(0)\right|}{(2p)!} 2^{2p} y^{2p}} dy = 0 \,. \tag{16}$$

This is a consequence of Theorem 2.1 in [Tug14a].

Proposition 4. Here, $d = 1$. We assume that ψ is quadratic: $\psi(x) := \frac{\alpha}{2}x^2$. Thus, for any $\alpha \geq 0$, there exists a critical value $\varepsilon_0(\alpha)$ such that Diffusion (3) admits a unique invariant probability provided that $\varepsilon > \varepsilon_0(\alpha)$.

This is a consequence of Proposition 2.4 in [Tug14a].

Theorem 4. *Let a_0 be a point where V admits a local minimum such that*

$$V(x) + F(x - a_0) > V(a_0) \quad \text{for all} \quad x \neq a_0 \,. \tag{17}$$

Then, for all $\kappa > 0$ small enough, there exists $\varepsilon_0 > 0$ such that $\forall \varepsilon \in]0; \varepsilon_0[$, the diffusion (3) *admits a stationary measure ρ_∞ satisfying*

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} ||q - a_0||^{2n} \rho_\infty(q,p) dq dp \leq \kappa^{2n} \,.$$

This is a consequence of Theorem 2.3 in [Tug14b].

More generally, all the results in [HT10a, HT10b, HT12, McK66, McK67, Tug10, Tug11, Tug14a, Tug14b] hold.

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